Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE LIBRARIES
Inventor(s): Stephan SCHUNK et al
Appl. No.: 09/876,142

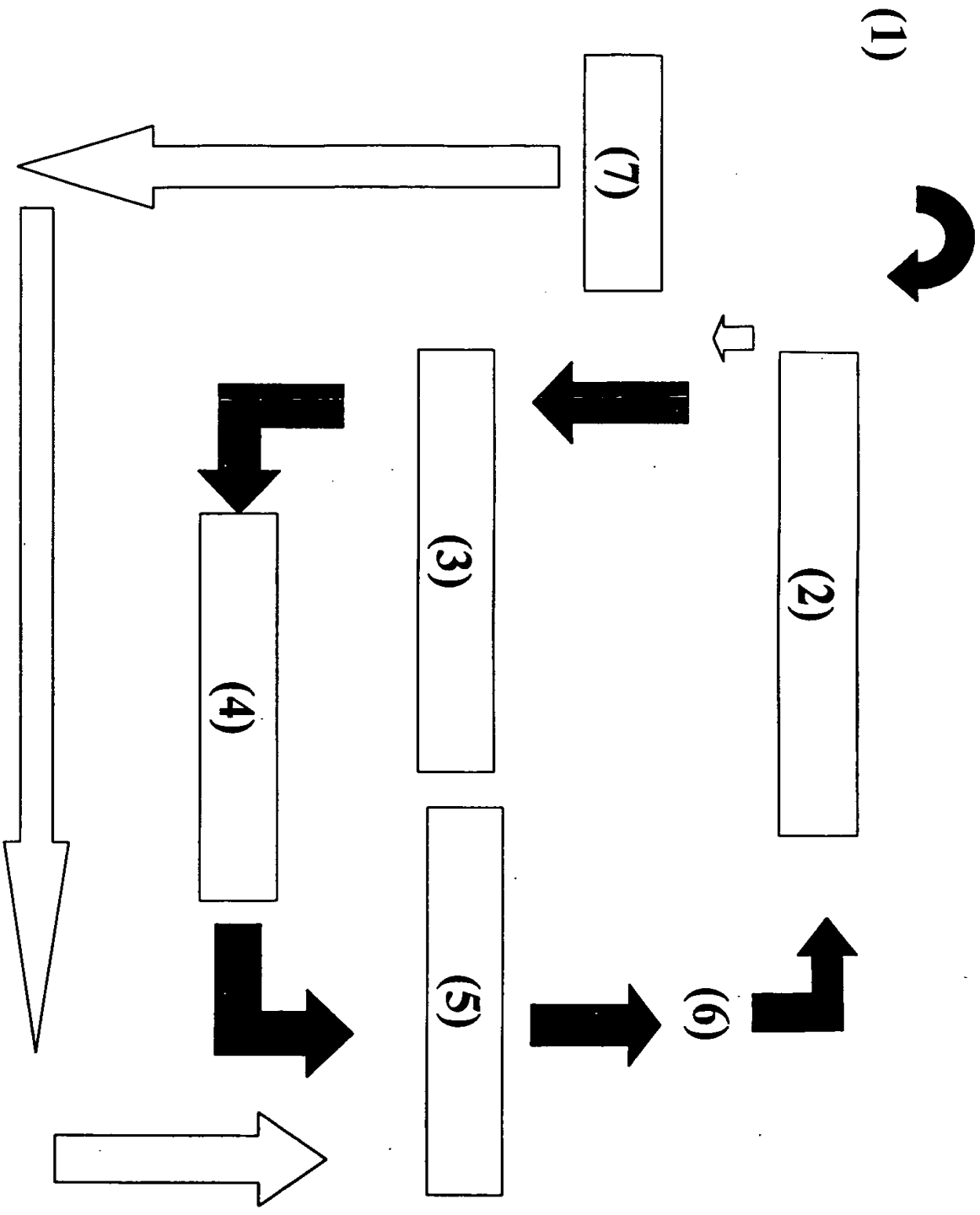

Fig. 1

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Performance Characteristics

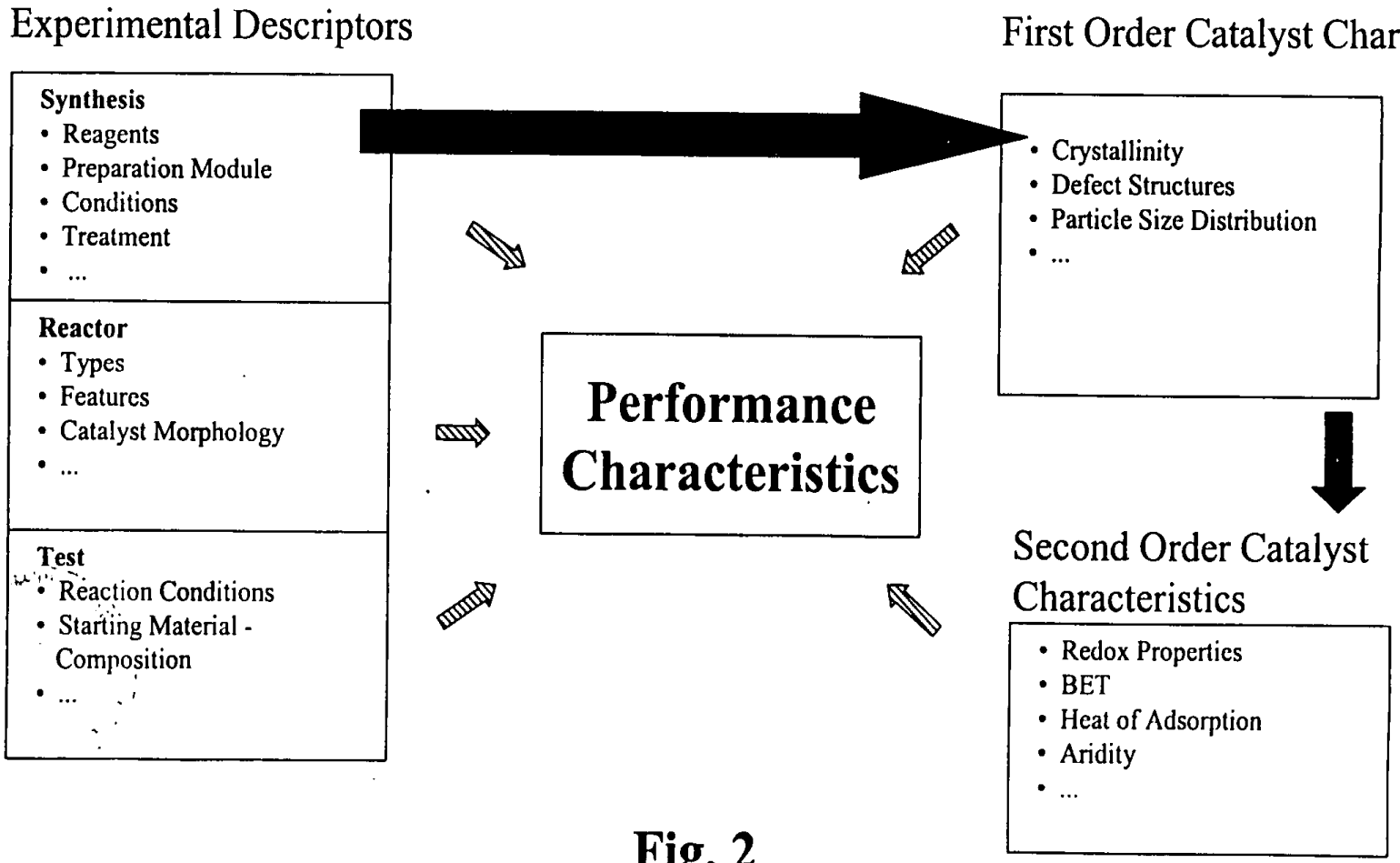

Fig. 2

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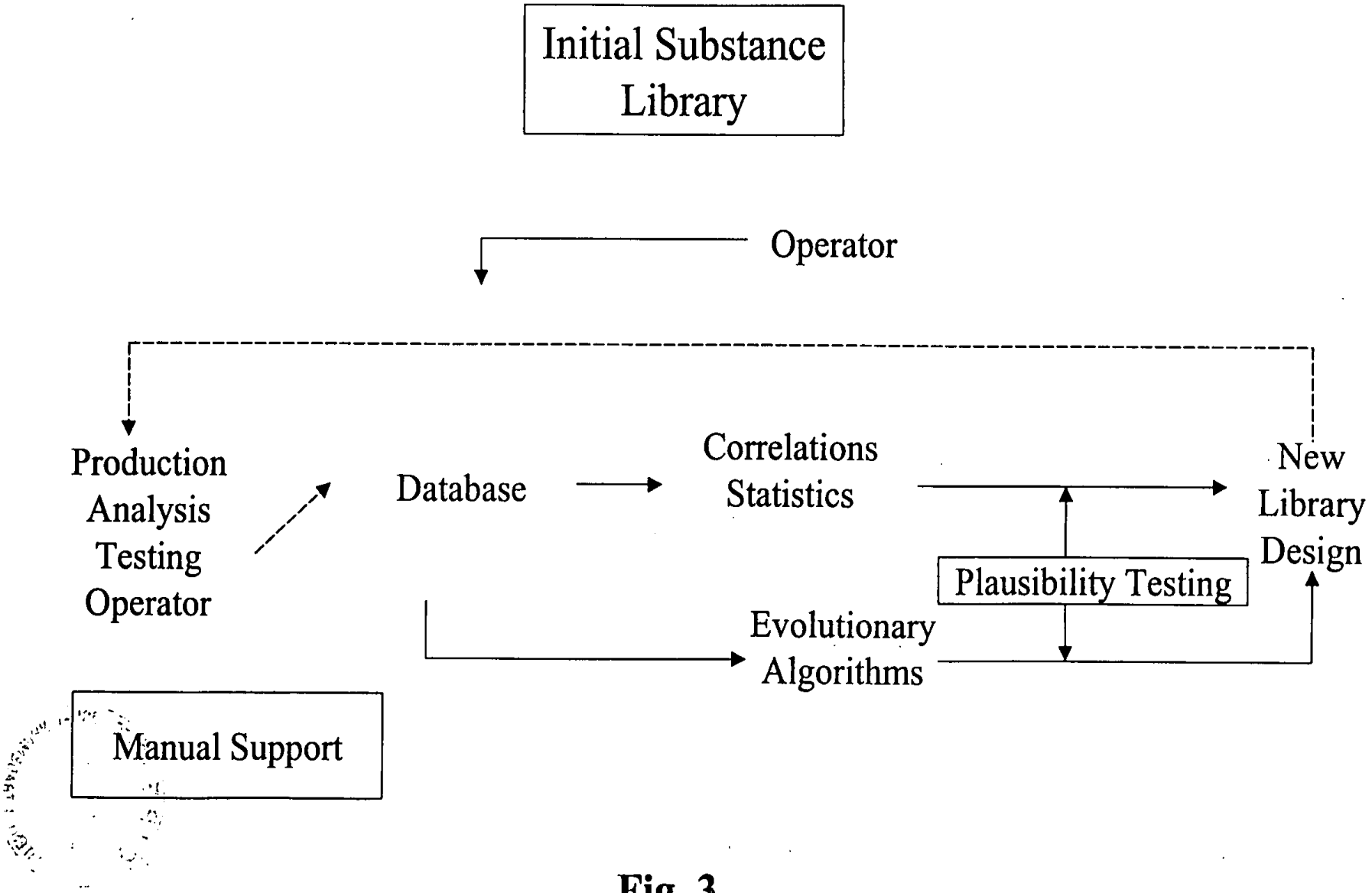

Fig. 3

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Fig. 4

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Original Library Design and Tests Using the Entire Parameter Space

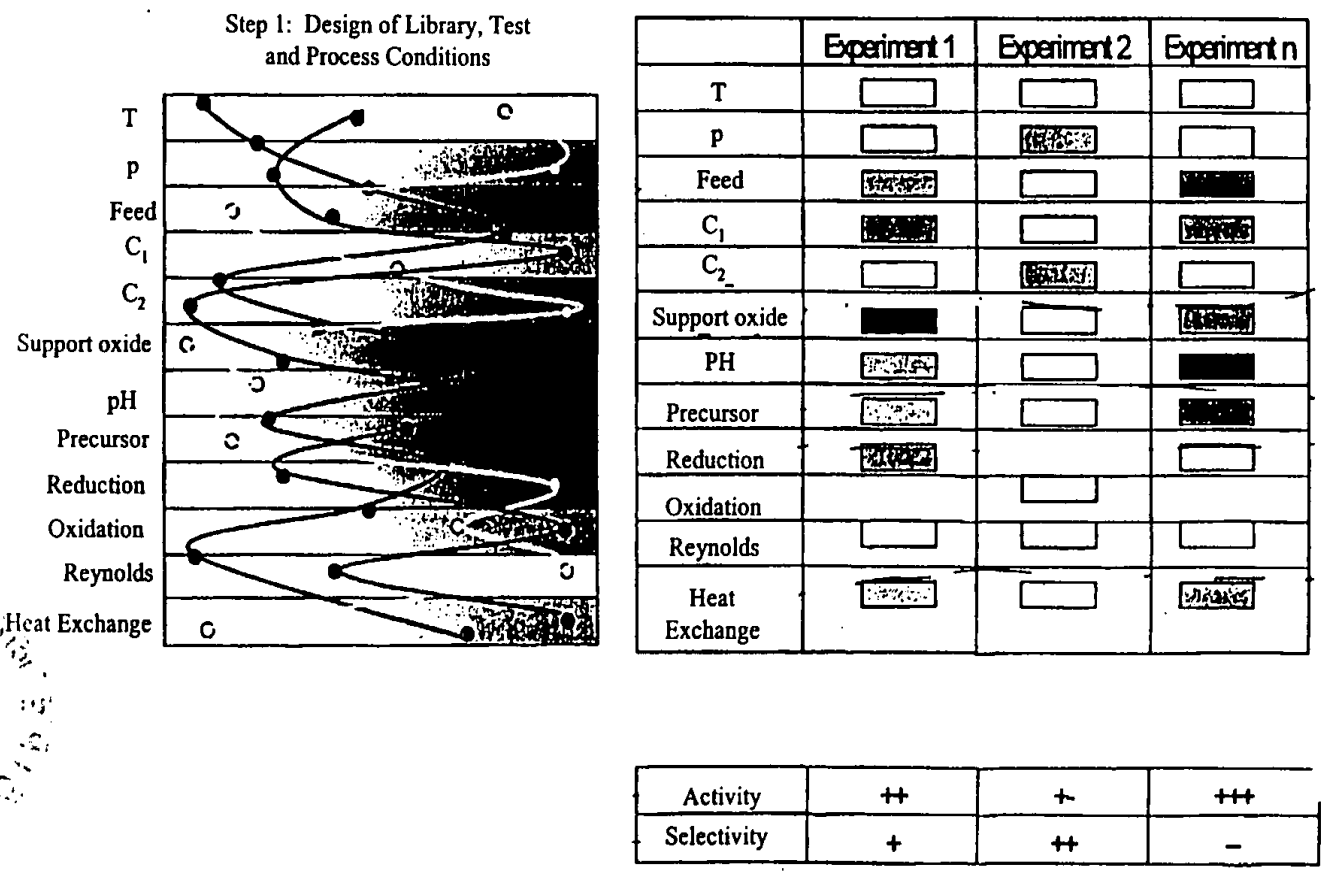

Fig. 5a

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Regression Analysis, Energies of the Parameter Space

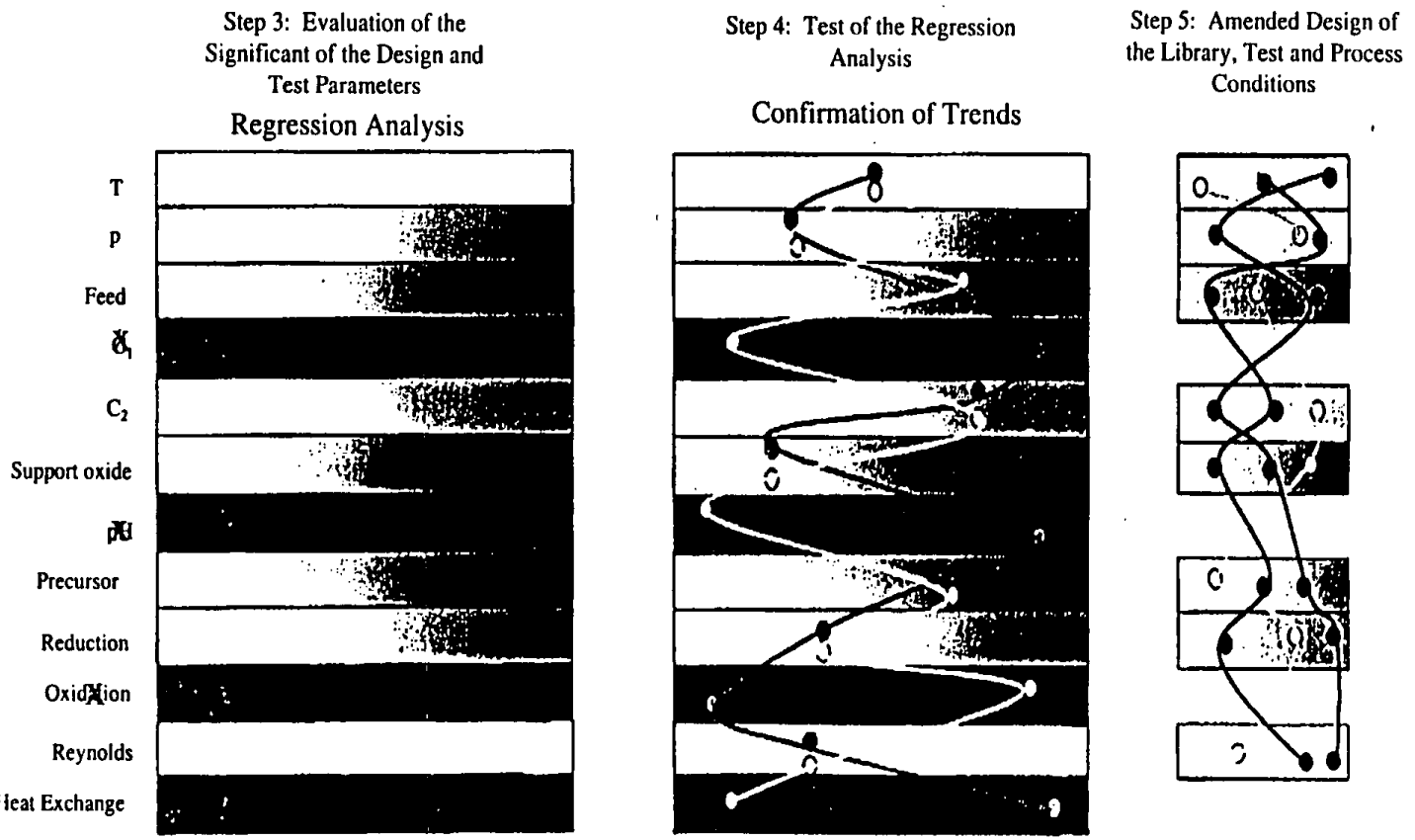

Fig. 5b

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Principle of Genetic Algorithms

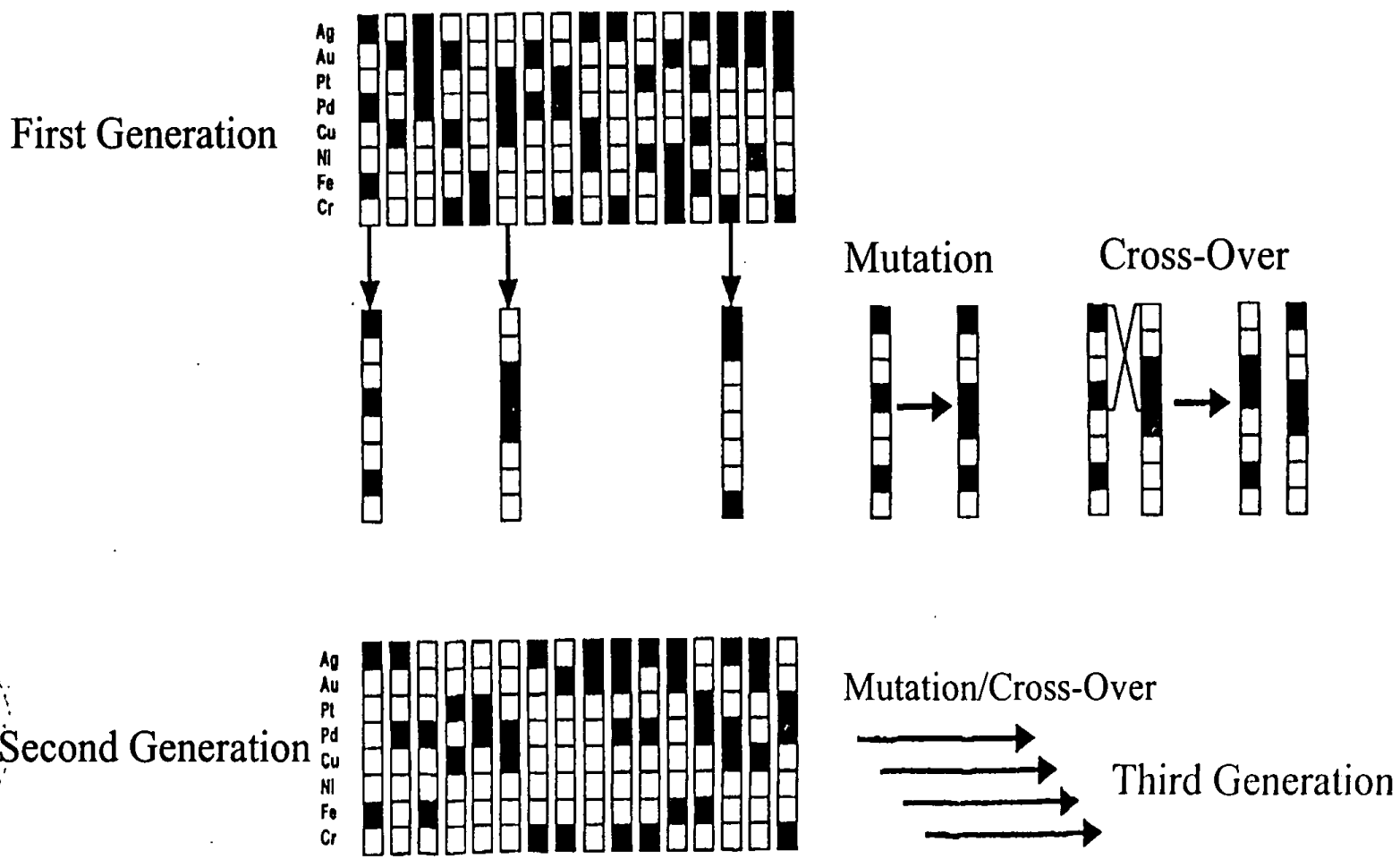

Fig. 5c

Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE LIBRARIES
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Sensitivity Analysis of the Parameters of the Initial Library Pareto Diagram

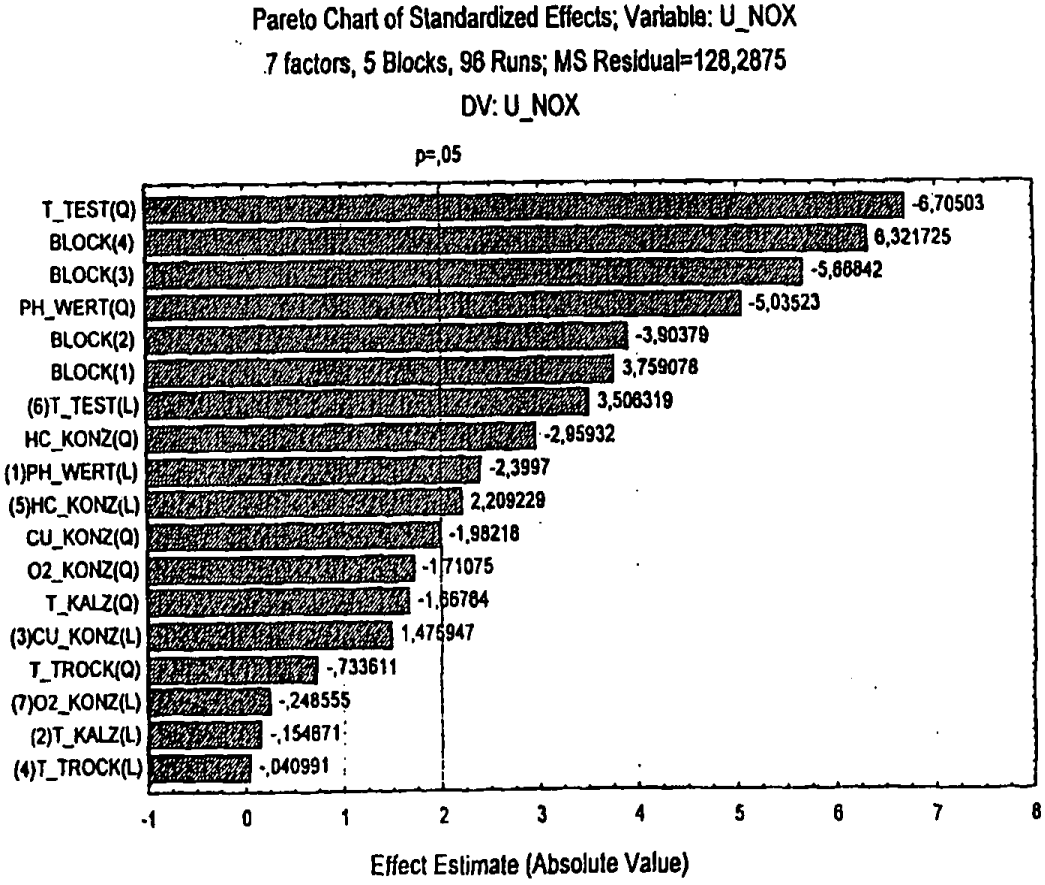

Fig. 6

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Sensitivity Analysis of the Parameters of the 1st Optimized Library Pareto Diagram

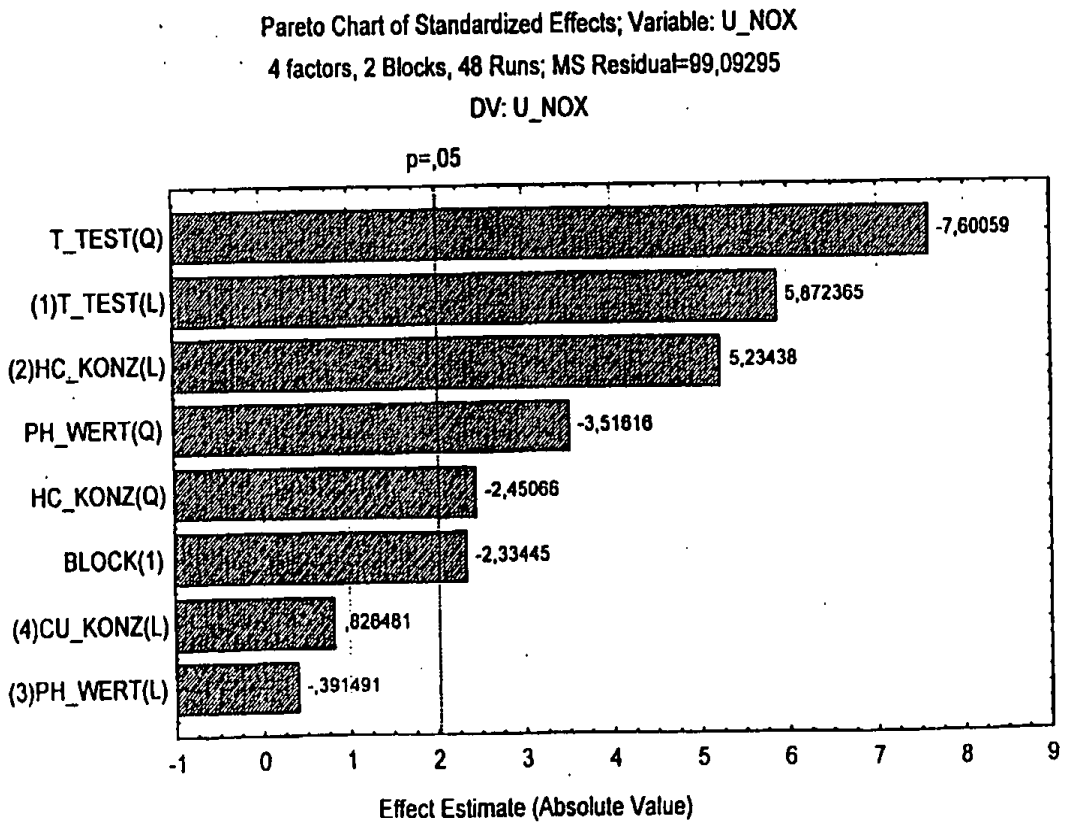

Fig. 7

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